

# Domain magnetization approach to the isothermal critical exponent

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We propose a method for calculating the isothermal critical exponent  $\delta$  in Ising systems undergoing a second-order phase transition. It is based on the calculation of the mean magnetization time series within a small connected domain of a lattice after equilibrium is reached. At the pseudocritical point, the magnetization time series attains intermittent characteristics and the probability density for consecutive values of mean magnetization within a region around zero becomes a power law. Typically the size of this region is of the order of the standard deviation of the magnetization. The emerging power-law exponent is directly related to the isothermal critical exponent  $\delta$  through a simple analytical expression. We employ this method to calculate with remarkable accuracy the exponent  $\delta$  for the square-lattice Ising model where traditional approaches, like the constrained effective potential, typically fail to provide accurate results.

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## I. INTRODUCTION

The statistical properties of interacting spins on the lattice are of fundamental importance for our understanding of equilibrium phase transitions in nature. Among them the most studied candidate is the Ising model [1, 2] in one, two, and three spatial dimensions finding application in a wide range of physical systems ranging from pure and random ferromagnets [3–7] to neurons [8, 9] and hadronic matter [10]. For  $D \geq 2$  spatial dimensions the usual Ising model for a lattice with infinite size possesses a thermal phase transition of second order, signaling the spontaneous symmetry breaking of mirror symmetry and the emergence of a ferromagnetic (for attractive spin-spin interaction) phase. This transition is characterized by the presence of a critical temperature  $T_c$  at which a scale-free behavior dominates the underlying phenomenology [11–13]. The absence of a characteristic scale at the critical point is related to the divergence of the correlation length  $\xi$  which in turn leads to the appearance of a variety of power laws with associated critical exponents. One of the main tasks in the study of models showing critical behavior is the determination of the values of these exponents which are then related to the respective universality classes.

For  $D = 2$  the Ising model with next-neighbor interactions is analytically solvable [14] while for  $D > 2$  one has to rely on numerical simulations and other approximate type of solutions for its study, see e.g. [6, 7] and references therein. Employing numerical methods constrains the mathematical analysis on lattices with finite size introducing an additional scale in the problem. This adds a complication in the development of methods to calculate the critical temperature as well as the critical exponents, usually solved by the so called finite-size scaling analysis [11–13]. This requires the determination of observables in lattices of increasing size in order to ex-

trapolate to the infinite size limit. Coming back to the 2D Ising model, despite of being analytically solvable, it offers a playground for testing a variety of simulation algorithms [6] and in fact a very hard one, since its finite-size scaling analysis possesses severe peculiarities due to the presence of significant, non-universal, logarithmic corrections [15, 16].

A dominant feature of the critical state in Ising-like systems, consequence of the absence of a characteristic length scale, is the formation of self-similar ordered clusters of spins with fractal geometry. The associated fractal dimension of the resulting set of ordered clusters is related to the isothermal critical exponent  $\delta$  which in turn determines the universality class of the undergoing transition. Thus, the calculation of the exponent  $\delta$  is a very significant task in the simulations of critical systems. Usually, in order to obtain the value of the exponent  $\delta$  one can either calculate the fractal dimension of the ordered clusters at  $T_c$  [17] or estimate the so called constrained effective potential [18]. For lattices with finite sizes the fractal geometry is an approximate property expressed through self-similar structure between two scales, the constrained effective potential acquires finite volume corrections and the critical temperature is replaced by the pseudocritical one, making the related analysis a highly non-trivial task. Nevertheless the aforementioned methods work quite well for the case of the 3D Ising model [19]. However they practically fail to give the right answer in the 2D case since they suffer from the presence of large finite-size corrections, that are hard to control.

In the present work we develop a method to calculate the critical exponent  $\delta$  for Ising systems based on properties of the magnetization time series after thermal equilibrium is reached. The idea is to consider the mean magnetization time series obtained by averaging over a connected small subset of the lattice. The main advantage of considering such small domains relies on

the fact that the number of the microstates determining their thermodynamic properties decreases exponentially with decreasing domain size. Thus, for small domains a much better covering of the available phase space can be achieved. On the other hand the domains are always open systems and therefore their thermodynamic properties are quite different from those of the entire (closed) lattice. Based on the distribution of the mean magnetization values within such a small domain one observes that each domain equilibrates at its own effective temperature. In fact with decreasing size the effective temperature decreases too. The method of analysis of the domain magnetization time series at equilibrium makes use of fact that for a closed system the distribution of waiting times in the neighborhood of the “false” vacuum, exhibiting the spontaneous symmetry breaking, is known for temperatures  $T \lesssim T_c$ . Namely at  $T = T_c$  the distribution is a power law with an exponent directly related to the isothermal critical exponent  $\delta$  [20], while for  $T < T_c$  the power law gets gradually destructed and exponential tails appear. However, for small to moderate waiting times the power-law description is still valid and the connection to  $\delta$  holds too [21].

We use here this information to extract the isothermal critical exponent  $\delta$  for an Ising system. Our basic assumption, validated by our numerical results, is that the waiting-time distributions derived in Refs. [20, 21] are valid also for an open Ising spin system in a thermal environment. Thus, we consider an ensemble consisting of domains of increasing size, parts of an Ising lattice at the corresponding (pseudo)critical temperature. For each such domain we calculate the mean magnetization as a function of time for a long time interval. Time is measured in single spin flips of the entire lattice. Based on this time series we calculate the distribution of waiting times in the neighborhood of  $\langle M_{\mathcal{D}_i} \rangle = 0$  for each domain  $\mathcal{D}_i$  and from these distributions we determine  $\delta$ . For very small domains the corresponding effective temperature is also extremely small and the distribution of the waiting times becomes pure exponential containing no information for the critical exponent  $\delta$ . Thus we use a cutoff on the minimum size of the considered domains. We apply this approach to the 2D Ising model on the square lattice with nearest-neighbor interactions and we obtain a highly accurate estimate for  $\delta$ . Since the developed method is quite general, it can in principle be applied to a wide class of spin lattices in two, but also higher dimensions.

The rest of paper is organized as follows: In Sec. II we present the general strategy and the method of analysis employed to calculate  $\delta$  for arbitrary spin models of Ising type on the lattice. In Sec. III we apply the proposed method to the case of the 2D Ising model on the square lattice and we discuss the obtained results. Finally, our concluding remarks are presented in Sec. IV.

## II. STRATEGY AND METHOD OF ANALYSIS

We consider the fluctuations of the magnetization for a spin model of the typical Ising form at thermal equilibrium defined by the Hamiltonian [7]

$$\mathcal{H} = - \sum_{\langle i,j \rangle} J_{ij} s_i s_j, \quad (1)$$

where as usual  $s_i = \pm 1$  and  $\sum_{\langle i,j \rangle}$  indicates summation over nearest neighbors. The condition  $J_{ij} > 0$  restricts the following considerations to the ferromagnetic case, although most of the obtained results are expected to hold more generally. We are interested for the time evolution of the magnetization calculated in a connected compact domain  $\mathcal{D}$ , subset of the entire lattice. Thus, the observable we focus on is defined via

$$M_{\mathcal{D}}^{(L_d)}(n) = \sum_i s_i(n) \chi_{\mathcal{D}}(i); \quad \chi_{\mathcal{D}}(i) = \begin{cases} 1; & i \in \mathcal{D} \\ 0; & i \notin \mathcal{D} \end{cases} \quad (2)$$

$L_d$  counts the number of sites in  $\mathcal{D}$  and  $n$  is the time unit measured in the minimum time needed for the flip of a single spin. Clearly  $1 \leq \ell \leq N_L$  where  $N_L$  is the total number of sites of the lattice. When  $\ell$  approaches  $N_L$  then  $M_{\mathcal{D}}^{(L_d)}(n)$  approaches the total magnetization of the spin lattice  $M_L$ . An important property of the magnetization time series is that it carries information of the approach to criticality, clearly manifested during relaxation in the effect of critical slowing down [6]. However, the imprints of criticality are present also to the post-equilibrium dynamics, as demonstrated in Ref. [20]. It is the latter information we will use in the present approach. In fact it is based on the observation that close to the critical point the magnetization time series becomes *sticky* in the neighborhood of the minimum of the effective potential of the magnetization which undergoes the spontaneous symmetry breaking. This behavior resembles intermittent dynamics close to a bifurcation [22].

Let us assume that local equilibrium, i.e. equilibrium with the domain  $\mathcal{D}$ , is reached before the establishment of global equilibrium. Then, after reaching global equilibrium, the domain magnetization time series  $M_{\mathcal{D}}^{(L_d)}(n)$  fluctuates around a stationary mean value. The fluctuations define a probability distribution  $P_{\mathcal{D}} = P_{\mathcal{D}}[M_{\mathcal{D}}^{(L_d)}]$  characteristic for the considered domain. For a periodic lattice the exact position of the domain is irrelevant and the distribution  $P_{\mathcal{D}}$  depends only on the size of  $\mathcal{D}$ . In fact each domain of different size is characterized by a different probability distribution  $P_{\mathcal{D}}$  at equilibrium. This is quite plausible since pseudocritical temperatures calculated for lattices of different size increase with decreasing lattice size. According to this reasoning the pseudocritical temperature of the entire lattice will be equivalent to an effective temperature below the pseudocritical one for smaller domains embedded in the lattice. This can be clearly seen in the distribution  $P_{\mathcal{D}}$  which is expected to attain the spontaneously broken form for each such domain.

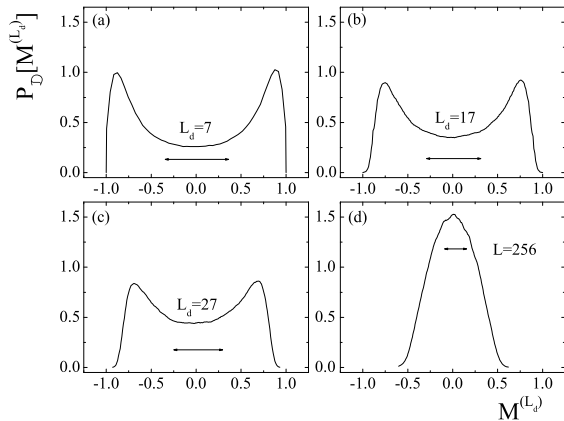


FIG. 1: Normalized magnetization probability distribution at the pseudocritical temperature  $T_c = 2.29$  calculated in  $L_d \times L_d$  domains of a square Ising lattice with linear size  $L = 256$  for various values of  $L_d$ : (a)  $L_d = 7$ , (b)  $L_d = 17$ , and (c)  $L_d = 27$ . In panel (d) the corresponding distribution for the entire lattice is shown. In each plot the arrows indicate the half-variance region around the mean value  $M = 0$  used in the calculation of the waiting-time distribution.

Concerning criticality the main claim of the present work is that one can use the time series  $M_D^{(L_d)}(n)$  (leading to  $P_D$  is the post-equilibrium phase) to decode information related to the isothermal critical exponent  $\delta$ . Based on  $M_D^{(L_d)}(n)$  it is straightforward to calculate the waiting times  $\tau^{(L_d)}$  in the neighborhood of the false vacuum at  $M_D^{(L_d)} = 0$ . There is no strict definition of the term “neighborhood” here and the half of the variance of the distribution  $P_D$  can be used as a typical neighborhood size. As shown in Ref. [20], for a finite system of size  $L$  at the pseudocritical temperature  $T_c$  the distribution of the waiting times  $\rho_{L,c}(\tau)$  has the form

$$\rho_{L,c}(\tau) = c_L \tau^{p_2(L)} e^{-p_3(L)\tau}, \quad (3)$$

where  $c_L$  is a normalization factor and  $p_2(L)$ ,  $p_3(L)$  are associated characteristic exponents. For an infinite system  $p_3(\infty) \rightarrow 0$  and Eq. (3) becomes a pure power law with  $p_2(\infty) \rightarrow \frac{\delta+1}{\delta}$ . Thus the exponent  $p_2$  encodes information of the isothermal critical exponent  $\delta$ . Interestingly enough, this information is also encoded in the waiting-time distribution around the false vacuum just after the spontaneous symmetry breaking [21]. The corresponding distribution  $\rho_{L,bc}(\tau)$  attains the form

$$\rho_{L,bc}(\tau) = \tilde{C}_L \frac{e^{\tau(\zeta(L)-1)(r(L)-1)}}{[e^{\tau(\zeta(L)-1)(r(L)-1)} - 1]^{\frac{\zeta(L)}{\zeta(L)-1}}}, \quad (4)$$

where  $\zeta(L)$  and  $r(L)$  are further characteristic exponents. Note that in both Eqs. (3) and (4) above, the underscripts  $c$  and  $bc$  refer to critical and below critical regimes. For an infinite system  $\zeta(\infty) = \delta + 1$  while  $r(\infty)$  tends to

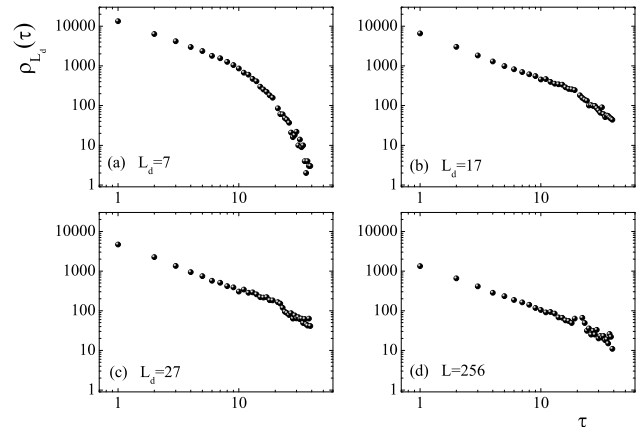


FIG. 2: The probability distribution of the waiting times in the neighborhood of  $M = 0$  [indicated by the arrows in Fig. 1(a) - (d)] at the pseudocritical temperature  $T_c = 2.29$  for square domains with linear sizes: (a)  $L_d = 7$ , (b)  $L_d = 17$ , (c)  $L_d = 27$ , and (d) for the entire lattice. Note that for the panels (a), (b), and (c),  $\rho_{L_d}(\tau) \equiv \rho_{L_d,bc}(\tau)$ , whereas for panel (d)  $\rho_{L_d}(\tau) \equiv \rho_{L_d,c}(\tau)$ .

a non-universal finite value greater than 1. For small  $\tau$  the density  $\rho_{L,bc}$  behaves as a power law  $\sim \tau^{-\frac{\zeta(L)}{\zeta(L)-1}}$  while for large  $\tau$  it decays exponentially  $\sim e^{\tau(r-1)}$ . Thus Eq. (4) can be used to estimate  $\delta$  for  $T \lesssim T_c$ . This task will be fulfilled in the next Section. Using a set of coexisting domains  $\mathcal{D}_i$  of different sizes  $L_d^{(i)}$  embedded in an Ising lattice, we will first determine the waiting-time distribution  $\rho_{L_d^{(i)},bc}(\tau)$  for each such domain. Then fitting the resulting distribution with a power law in the small  $\tau$  region we will determine the exponent  $\zeta(L)$  and subsequently the isothermal critical exponent  $\delta$ . The main assumption here is that each domain can be considered as an Ising lattice of smaller size than the size of the lattice it is embedded into. The Ising spins of the entire lattice, not belonging to the considered domain, form a thermal environment for this domain at a temperature which depends on the domain size  $L_d^{(i)}$ . There is a good reason for adopting this scenario: as it will be demonstrated in the next Section the properties of small domains are obtained with much higher accuracy than those of the larger domains probably due to an exponentially better covering of the corresponding microstate space. This leads to a robust estimation of the isothermal exponent  $\delta$ . Of course the size of the domains should not arbitrarily decrease since in this case Eq. (4) is not valid any more.

### III. RESULTS FOR THE 2D ISING MODEL

We apply the method of analysis described in the previous Sec. II on the square-lattice Ising model attempting to calculate the isothermal critical exponent  $\delta$ . In

the Hamiltonian of Eq. (1) we use the homogeneous case  $J_{ij} = J$  for all pairs  $i$  and  $j$ . We investigated the equilibrium dynamics of the Ising spins, mainly for a lattice set-up with linear size  $L = 256$ .

In the pre-equilibrium phase the spin dynamics is simulated using the Wolff's cluster algorithm [23], which is a variant of the original Swendsen-Wang algorithm [24], for reasons that are exemplified below. In the Swendsen-Wang algorithm, small and large clusters are created. While the destruction of critical correlations is predominantly due to the large clusters, a considerable amount of effort is spent on constructing the smaller clusters. In Wolff's implementation, no decomposition of the entire spin configuration into clusters takes place. On the contrary, only a single cluster is formed, which is then always flipped. If this cluster turns out to be large, correlations are destroyed as effectively as by means of the large clusters in the Swendsen-Wang algorithm, without the effort of creating the smaller clusters that fill up the remainder of the lattice. If the Wolff cluster turns out to be small, then not much is gained, but also not much computational effort is required. As a result, critical slowing down using the Wolff implementation is suppressed even more strongly than in the Swendsen-Wang case.

After reaching equilibrium, a hybrid algorithm is employed involving mainly single spin flips mixed with rare Wolff's steps to increase ergodicity. The latter is reflected in the smooth form obtained for the magnetization histograms. Actually the obtained results are robust against changes of the simulation algorithm provided that time is expressed in single spin flips. Thus, for example, employing Wolff's cluster algorithm one has to take into account the size of the cluster when assigning a characteristic time to the cluster flipping. This increases the corresponding waiting times.

In our calculations we used square domains of linear sizes  $L_d = 7, 13, \dots, 27$ . The pseudocritical temperature  $T_c \approx 2.29$  is estimated through the magnetization histogram as the minimum temperature for which symmetry breaking is not yet globally established. In Fig. 1(a) - (d) we show the magnetization probability distribution for domains with  $L_d = 7, 17, 27$  as well as for the entire lattice  $L = 256$ . In each case it is calculated using a time series of  $10^6$  steps after reaching equilibrium. In accordance with the discussion in Sec. II we clearly observe that the magnetization distribution for decreasing linear size corresponds to a spin system with decreasing temperature. The arrows indicate the half-variance region around the  $M = 0$  value.

In Fig. 2(a) - (d) we show the corresponding distribution of the waiting times  $\tau$  in the half-variance region indicated in Fig. 1(a) - (d). We clearly observe the power-law behavior for low  $\tau$ -values when  $L_d \geq 17$ . For  $L_d = 7$  the effective temperature in the domain is far below the pseudocritical one corresponding to this lattice size [see the distribution in Fig. 1(a)] and therefore no power-law behavior is clearly observed. Nevertheless a fit using the form dictated by Eq. (4) works still sufficiently well, pro-

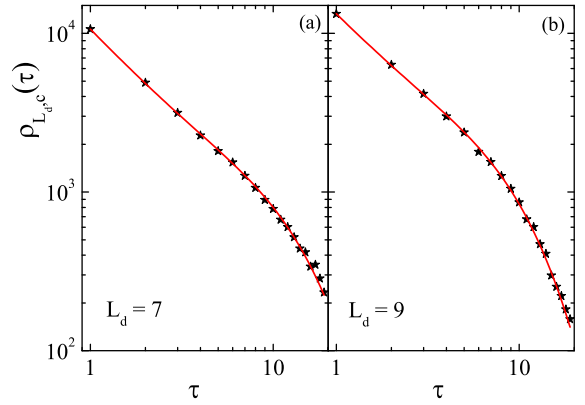


FIG. 3: (color online) The distribution  $\rho_{L_d,c}(\tau)$  shown by stars for (a)  $L_d = 7$  and (b)  $L_d = 9$  in a double-logarithmic scale. In both panels the red solid line illustrates the fitting result obtained using the function of Eq. (4).

viding a reasonable value for the exponent  $\zeta$ . This is demonstrated in Fig. 3, where we plot with stars the distribution  $\rho_{L_d,c}(\tau)$  for  $L_d = 7$  (a) and  $L_d = 9$  (b), respectively. The corresponding fitting results are shown by the red solid lines in the two panels. They lead to  $\zeta(L_d) \approx 4.3$  for both values of  $L_d$ . As the size of the domain decreases, the exponential tail dominates more and more, extending also to the low- $\tau$  region and the power-law behavior gradually disappears. Therefore we do not consider domains with  $L_d < 7$ . For  $L_d > 10$  we fit the waiting-time distribution with a power law in the low- $\tau$  region ( $\tau < 20$ ) for each considered domain and we extract the exponent  $p_2(L_d) = \zeta(L_d)/[\zeta(L_d) - 1]$ . We check the validity of the power-law description by repeating the fit with the form given in Eq. (4) and comparing the obtained value of  $p_2(L_d)$  to the value found by the direct power-law fit. We observe that for  $L_d > 11$  the two values practically coincide.

In Fig. 4 we show graphically the results obtained for the characteristic exponent  $p_2(L_d)$  and for  $L_d \geq 9$ . We observe a rapid convergence to the value  $(\delta + 1)/\delta = 16/15 \approx 1.07$ , shown by the red solid line. For large domain sizes the errors increase due to the fact that the microstate space increases exponentially and therefore the statistical fluctuations in the calculation of the waiting time distribution increase too. The isothermal critical exponent  $\delta$  is estimated via  $\delta = \frac{1}{p_2(L_d) - 1}$ . For the 2D Ising model this calculation leads to the result  $\delta_{2D} = 14.7 \pm 1.4$  (obtained by a fit with a constant for  $L_d \geq 15$ ) which is in very good agreement with the exact value  $\delta_{2D} = 15$  [3, 16].

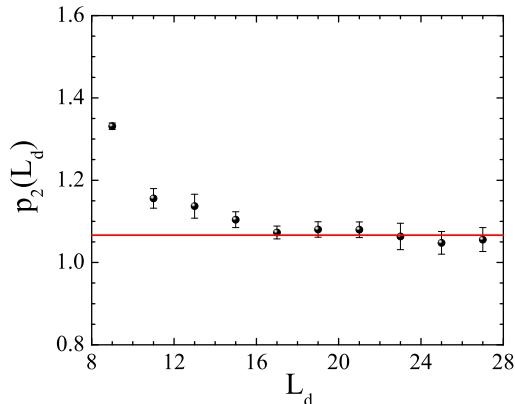


FIG. 4: (color online) The exponent  $p_2(L_d)$  calculated from the distributions  $\rho_{L_d}(\tau)$  as explained in the text. The red line is at  $16/15 \approx 1.067$  (analytical result).

#### IV. CONCLUDING REMARKS

We proposed an approach for the calculation of the isothermal critical exponent  $\delta$  in a spin lattice undergoing a second-order phase transition. Our method makes use of critical characteristics present in post-equilibrium spin dynamics as revealed in Refs. [20, 21]. In fact the effective magnetization dynamics close to the vacuum undergoing the spontaneous symmetry breaking is similar to intermittent dynamics close to a bifurcation. The information concerning  $\delta$  is encoded in the distribution of waiting times of the magnetization time series near the broken vacuum. The key ingredient of the method is the calculation of the magnetization time series within do-

main of varying size embedded in the spin lattice. These domains equilibrate locally to a lower temperature than that of the entire lattice. When this temperature is not too far from the pseudocritical one, then the waiting-time distribution carries information of the critical point related to  $\delta$ , as shown in Ref. [21]. Furthermore, it can be calculated with higher accuracy since the number of microstates of the smaller domain is exponentially reduced compared to that of the entire lattice. For small to moderate values of the waiting times, the associated distribution is a power law with an exponent which is related to  $\delta$  and can be estimated employing a suitable fitting procedure. Subsequently the sequence of the fitted exponents as a function of the increasing domain size can be used for an accurate determination of  $\delta$ . The proposed method has been applied to the 2D Ising model on the square lattice providing remarkably good results. Let us note here that our choice to use the 2D Ising ferromagnet as a platform model was dictated by the existence of an exact analytical result of the isothermal exponent, so that a direct comparison was possible. However, since the dynamical properties consisting the backbone of the method are universal, one expects that the method can be used in a wide class of spin systems to calculate the isothermal critical exponent in a rather straightforward manner.

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